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Resonant acceptors states in $Ge/Ge_{1-x}Si_x$ MQW heterostructures

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Abstract. New nonvariational theoretical approach allowing to calculate both the localized and the continuum states of charge carriers in QW heterostructures in the presence of the Coulomb potential has been developed. The method has been used to calculated the energy spectra of shallow acceptors in strained Ge/GeSi MQW heterostructures. Optical transitions from the acceptor ground states to the resonant states have been revealed in the measured far IR photoconductivity spectra of the heterostructures.

1. Introduction

In recent years there has been considerable interest to the resonant impurity states in semiconductors (see for example [1]). This interest was stimulated by the observation of stimulated emission of far infrared (FIR) radiation observed in uniaxially compressed p-Ge at high electric fields [1]. In uniaxially stressed p-Ge the resonant states arise due to the splitting of light and heavy hole subbands at high enough stress value when the impurity levels pertain to the upper split-off subband turn out in the energy continuum of the lower subband. The similar situation can be easily realized in quantum well (QW) heterostructures where the resonant acceptor states arise due to QW confinement. The paper is devoted to the theoretical and experimental study of the resonant acceptor states in strained Ge/GeSi(111) multiple-quantum-well (MQW) heterostructures.

2. Theoretical formalism

The new nonvariational approach has been developed for the calculation of the acceptors energy spectra. The spectra of shallow acceptors in Ge/GeSi QW heterostructures were calculated in the framework of the envelope function approximation. The acceptor Hamiltonian used was 4×4 matrix operator included Luttinger Hamiltonian, the deformation term, the QW confinement potential due to the valence band discontinuity and the Coulomb potential. Similar to the work [2] the axial approximation was used, i.e. the Hamiltonian was considered to be invariant by rotation about the $z \| [111]$ axis (the axis perpendicular to the growth plane of the structure). In this case the z-component of the total angular momentum J_z is a good quantum number and the acceptor states are two-fold degenerate by the sign of the component of the angular momentum [2]. The acceptor envelope function was expanded in the basis of free hole envelope functions in the QW $v_n^s(\mathbf{k}, z)e^{i\mathbf{k}\mathbf{r}_\parallel}$, which are eigenstates of the Hamiltonian not containing the Coulomb potential:

$$F^s(\mathbf{r}) = \sum_n \int d\mathbf{k} C_n(\mathbf{k}) v_n^s(\mathbf{k}, z) e^{i\mathbf{k}\mathbf{r}_\parallel} \tag{1}$$

where n is number of subband, $\mathbf{r}$ is radius-vector, $\mathbf{r}_{\|} = (r_{\|}, \theta)$ is the in-plane coordinate and $\mathbf{k} = (k, \alpha)$ is the hole wave vector. In the axial approximation the expansion coefficients take the following form:

$$C_n(\mathbf{k}) = C_n(k)\mathrm{e}^{im\alpha} \tag{2}$$

where m is the projection of the total angular momentum on the z-axis. By substituting the expansion (1) into the Schrödinger equation for the envelope function the integral equations for the above expansion coefficients were obtained. The integrals were approximated by the discrete sums over the hole momentum k, the step difference being chosen much less than the inverse Bohr radius. The sums were interrupted at k much greater than the inverse Bohr radius. Therefore the problem was reduced to the diagonalization of the finite symmetric matrix (typically 500 × 500). Using this method the energies and wave functions of states, which correspond to the values of total angular momentum projection $J_z = \pm 3/2$, $J_z = \pm 1/2$ and $J_z = \pm 5/2$ were calculated. Dipole optical transition from the acceptor ground state ($J_z = \pm 3/2$) are allowed into localized excited states and the states of the continuum corresponding to $J_z = \pm 1/2$ and $J_z = \pm 5/2$.

The acceptor wave functions have the complicated structure. Expansion (1) include terms referred to different hole subbands in the QW. If the expansion of a wave function mainly consists of free hole envelope functions of the certain subband, we'll ascribe the state corresponding to the function to this subband. The acceptor ground state pertains to the 1st subband hh1 and has a negative energy (with respect to the bottom of hh1 subband). The energy of a state pertaining to an upper subband can be either negative (localized state) or positive (resonant state). The localized state which pertains to an upper subband becomes resonant if the width of the quantum well is reduced. The part of the wave functions of resonant state consisting of the hole envelope functions of the subband to which this state is pertained to looks like the wave function of the similar localized state corresponding to 1st hole subband.

3. Results and discussion

Measured FIR photoconductivity spectra of undoped Ge/GeSi MQW heterostructure are shown in Fig. 1 by solid lines. The residual shallow acceptors concentration is estimated to be about $10^{14}\,\mathrm{cm}^{-3}$. In the long wavelength range (Fig. 1(a)) the photoconductivity results from the optical transitions from the acceptor ground state to the continuum and to the excited localized states (and subsequent thermoionization). The binding energies of shallow impurities in QW heterostructures are known to be dependents on the impurity position in the well. This is clearly seen in Fig. 2 for the acceptor ground state in the investigated heterostructure. The dashed line in Fig. 1(a) shows the photoconductivity spectrum calculated at the supposition that acceptors are uniformly distributed over QW (details of the procedure are described in [3]). One can see that in this spectrum the photoconductivity maximum corresponds to the binding energy of on-center acceptors at about 7.4 meV. This results from the fact that the impurities situated near QW center (about 50% of QW width) have nearly the same binding energy (Fig. 2, cf. [3]). However the measured spectrum has quite a different form. There is a strong photoconductivity band in the spectrum in between 2.5 and 5 meV (Fig. 1(a)). The short wavelength edge of this band just corresponds to the binding energy of the acceptors situated at the heterointerface (on-edge acceptor, see arrows 1b in Fig. 1, 2). So it is naturally to assume that in addition to the uniformly distributed over QW width acceptors there are some centers concentrated near the heterointerface. A heterointerface is known to be a source of point defects and the observed residual acceptors

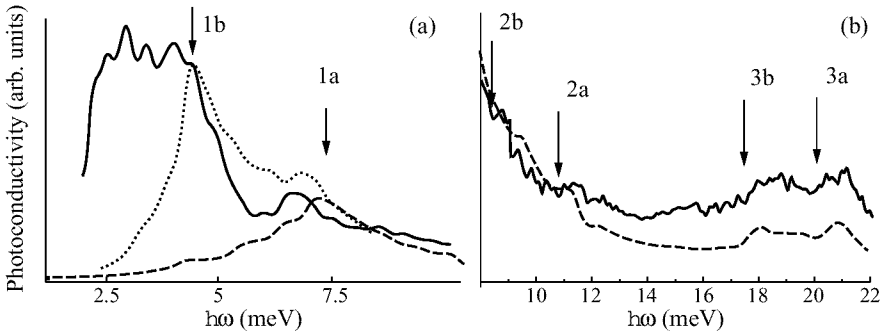

Fig. 1. Long (a) and short (b) wavelenght parts of the measured (solid line) and the calculated photoconductivity spectra of $Ge/Ge_{0.88}Si_{0.12}$ heterostructure #306 (d_{QW} = 200 Å, N_{QW} = 162, elastic deformation $\epsilon = 2.4 \times 10^{-3}$). Dashed and dotted lines correspond to two types of acceptor distribution over QW: uniform and uniform plus δ-layers at the heterointerfaces respectively. The sheet concentration at the heterointerfaces was taken half of that for the uniformly distributed acceptors per well. Arrows indicate binding energies for on-center (a) and on-edge (b) acceptors.

are likely to be connected with vacancies rather than with the chemical impurities. The dotted line in Fig. 1(a) represents the calculated photoconductivity spectra taking into account both the uniformly distributed and localized near heterointerfaces acceptors. It is clearly seen that the above model of the acceptor distribution describes fairly well both the photoconductivity peak at 7 meV and the short wavelength edge of the main photoconductivity band in between 2.5–5 meV. The long wavelength part of this band (that was observed in this particular sample only, cf. [4]) can be attributed to the photoionization either of the acceptors localized in barriers near heterointerfaces or of shallow A^+ centers in QWs [4].

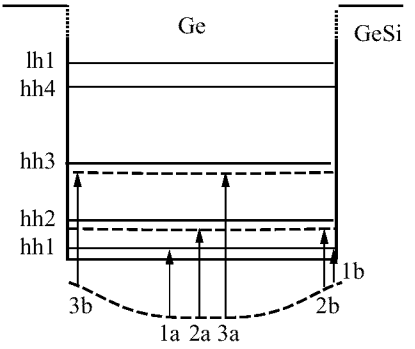

Fig. 2. Energy diagram of hole states in $Ge/Ge_{0.88}Si_{0.12}$ QW heterostructure #306. Solid and dashed lines correspond to free hole subbands (heavy holes: hh1–hh4, lidht holes: lh1) and acceptor levels (ground state and two "excited" resonant states). The arrows indicate the optical transitions introduced in the caption to Fig. 1.

The represented above approach allowed to calculate not only the localized acceptor states but all the states of the continuum including resonant states as well. The dotted curve in Fig. 1(b) shows the calculated spectrum of the photoconductivity resulted from the optical transitions from the acceptor ground state to the states of the continuum. To fit the spectral positions of the main features designated by arrows 3a and 3b in Fig. 1(b) to the experimentally observed ones we have to reduce the well width at the calculation down

to 185 Å (if compared with 200 Å obtained from X-ray analysis). Arrows 2a,b and 3a,b in Fig. 1(b), 2 indicate the optical transitions from the acceptor ground state $J_z = \pm 3/2$ to the "excited" resonant states ($J_z = \pm 1/2$ and $J_z = \pm 5/2$) pertained with the upper hole subbands hh2 (arrows 2) and hh3 (arrows 3) respectively for the on-center (a) and on-edge (b) acceptors. There are no doubts that the doublet 3a-3b really presents in the measured spectra in Fig. 1(b). Moreover there are noticeable spectral features in between 9–12 meV in the measured spectra that can be attributed to the doublet 2a-2b. To the authors knowledge this is the first observation of the resonant acceptor states in QW heterostructures.

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